Supporting Information

For

Palladium(II) thiocarboxamide complexes: Synthesis, characterisation and application to catalytic Suzuki coupling reactions

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^{1}H NMR spectral data for the coupling compounds:

4-Methoxybiphenyl: NMR ($CDCl_3$): δ_H (400 MHz) 7.46 (t, J = 8.8 Hz, 4H), 7.33 (t, J = 7.6 Hz, 2H), 7.24-7.20 (m, 1H), 6.90 (d, J = 8.8 Hz, 2H), 3.77(s, 3H) ppm.

4-Chloro-4'-methoxybiphenyl: NMR ($CDCl_3$): δ_H (400 MHz) 7.48-7.44 (m, 2H), 7.33 (t, J =7.2 Hz, 2H), 7.17 (d, J = 8.8 Hz, 2H), 6.90 (d, J = 8.8 Hz, 2H), 3.77 (s, 3H) ppm.

4'-Methoxy-4-methylbiphenyl: NMR ($CDCl_3$): δ_H (400 MHz) 7.45 (d, J = 8.0 Hz, 4H), 7.33 (d, J = 7.2 Hz, 2H), 6.90 (d, J = 8.0 Hz, 2H), 3.77 (s, 3H), 2.24 (s, 3H) ppm.

4, 4'-Dimethoxybiphenyl: NMR ($CDCl_3$): δ_H (400 MHz) 7.53 (t, J = 8.0 Hz, 2H), 7.43 (t, J = 7.2 Hz, 1H), 7.37 (d, J = 8.8 Hz, 2H), 6.97(d, J = 8.8Hz, 1H), 6.77(d, J = 9.2 Hz, 2H), 3.77 (s, 6H) ppm.

4-Methylbiphenyl: NMR ($CDCl_3$): δ_H (400 MHz) 7.96 (d, J = 8.4 Hz, 2H), 7.62-7.54 (m, 4H), 7.54-7.34 (m, 2H), 7.32 (t, J = 7.6 Hz, 1H), 2.31 (s, 3H) ppm.

4-Chloro-4'-methylbiphenyl: NMR ($CDCl_3$): δ_H (400 MHz) 8.21-8.19 (m, 2H), 7.65-7.63 (m, 2H), 7.46-7.44 (m, 2H), 7.23-7.18 (m, 2H), 2.34 (s, 3H) ppm.

4, 4'-Dimethylbiphenyl: NMR ($CDCl_3$): δ_H (400 MHz) 7.41-7.34 (m, 4H), 7.17-7.13 (m, 4H), 2.30 (s, 6H) ppm.

4-Methoxy-4'-methylbiphenyl: NMR ($CDCl_3$): δ_H (400 MHz) 7.41-7.34 (m, 4H), 7.24-7.13 (m, 4H), 3.76 (s, 3H), 2.31 (s, 3H) ppm.

5'-methyl-1,1':3',1"-terphenyl: NMR ($CDCl_3$): δ_H (400 MHz) 7.95 (d, J = 8.0 Hz, 2H), 7.74-7.54 (m, 6H), 7.41-7.32 (m, 5H), 2.31 (s, 3H) ppm.

4,4"-dichloro-5'-methyl-1,1':3',1"-terphenyl: NMR ($CDCl_3$): δ_H (400 MHz) 7.60-7.51 (m, 4H), 7.44-7.24 (m, 4H), 6.98-6.76 (m, 3H), 2.31 (s, 3H) ppm.

4,4",5'-trimethyl-1,1':3',1"-terphenyl: NMR ($CDCl_3$): δ_H (400 MHz) 7.39 (d, J = 8.4 Hz, 4H), 7.33 (t, J = 8.4 Hz, 4H), 7.08 (d, J = 8.8 Hz, 2H), 6.68 (d, J = 8.8 Hz, 1H), 2.37 (s, 3H), 2.34 (s, 6H) ppm.

4,4"-dimethoxy-5'-methyl-1,1':3',1"-terphenyl: NMR ($CDCl_3$): δ_H (400 MHz) 7.40-7.37 (m, 4H), 7.28 (d, J = 8.0Hz, 4H), 6.88 (d, J = 8.8 Hz, 2H), 6.69 (d, J = 8.8 Hz, 1H), 3.75 (s, 6H), 2.31 (s, 3H) ppm.

2-Phenylpyridine: NMR ($CDCl_3$): δ_H (400 MHz) 8.21 (d, J = 7.6 Hz, 1H), 7.65 (d, J = 7.6 Hz, 3H), 7.46 (d, J = 7.2 Hz, 3H), 7.21 (t, J = 8.0 Hz, 2H) ppm.

2-(4'-Chlorophenyl)pyridine: NMR ($CDCl_3$): δ_H (400 MHz) 8.04 (d, J = 8.8 Hz, 2H), 7.69 (d, J = 8.8 Hz, 2H), 7.64 (d, J = 8.8 Hz, 2H), 7.42 (t, J = 8.4 Hz, 2H) ppm.

2-(4'-Methylphenyl)pyridine: NMR ($CDCl_3$): δ_H (400 MHz) 8.05 (d, J = 7.2 Hz, 1H), 7.81 (d, J = 8.0 Hz, 1H), 7.67-7.55 (m, 4H), 7.23 (d, J = 9.6 Hz, 2H), 2.31 (s, 3H) ppm.

2-(4'-Methoxyphenyl)pyridine: NMR ($CDCl_3$): δ_H (400 MHz) 8.30-8.07 (m, 4H), 7.39 (d, J = 8.0 Hz, 2H), 6.93 (d, J = 8.0 Hz, 2H), 3.80 (s, 3H) ppm.

5-Methyl-2-phenylpyridine: NMR ($CDCl_3$): δ_H (400 MHz) 8.51 (s, 1H), 7.97-7.94 (m, 2H), 7.75-7.62 (m, 3H), 7.45 (d, *J* =7.6 Hz, 2H), 2.37 (s, 3H) ppm.

2-(4'-Chlorophenyl)-5-Methylpyridine: NMR ($CDCl_3$): δ_H (400 MHz) 8.43 (s, 1H), 7.82 (d, *J* = 8.4 Hz, 2H), 7.51 (t, *J* = 8.0 Hz, 2H), 7.40 (d, *J* = 8.4Hz, 2H), 2.30 (s, 3H) ppm.

2-(4'-Methylphenyl)-5-Methylpyridine: NMR ($CDCl_3$): δ_H (400 MHz) 8.49 (s, 1H), 7.65-7.63 (m, 2H), 7.46-7.44 (m, 2H), 7.22 (d, *J* = 8.0 Hz, 2H), 2.37 (s, 3H), 2.34 (s, 3H) ppm.

2-(4'-Methoxyphenyl)-5-Methylpyridine: NMR ($CDCl_3$): δ_H (400 MHz) 8.40 (s, 1H), 7.41-7.34 (m, 4H), 7.15 (d, *J* = 9.2 Hz, 3H), 3.76 (s, 3H), 2.30 (s, 3H) ppm.

2, 6-Diphenylpyridine: NMR ($CDCl_3$): δ_H (400 MHz) 7.95 (d, *J* = 8.4 Hz, 2H), 7.62-7.54 (m, 6H), 7.41-7.32 (m, 5H) ppm.

2, 6-Bis-(4'-chlorophenyl)pyridine: NMR ($CDCl_3$): δ_H (400 MHz) 7.94 (d, *J* = 8.4 Hz, 2H), 7.60-7.53 (m, 4H), 7.40-7.36 (m, 5H) ppm.

2, 6-Bis-(4'-methylphenyl)pyridine: NMR ($CDCl_3$): δ_H (400 MHz) 7.75 (d, *J* = 8.8Hz, 4H), 7.53 (d, *J* = 8.4 Hz, 4H), 7.40-6.94 (m, 3H), 2.31 (s, 6H) ppm.

2, 6-Bis-(4'-methoxyphenyl)pyridine: NMR ($CDCl_3$): δ_H (400 MHz) 7.89-7.86 (m, 2H), 7.41-7.38 (m, 4H), 7.28-7.26 (m, 1H), 6.89 (t, *J* = 8.8 Hz, 4H), 3.77 (s, 6H) ppm.

Table S1: Elemental Analysis data for Pd(II) thiocarboxamide complexes

Complexes	Empirical Formula	Calculated (Found)			
		C%	H%	N%	S%
[Pd(Cl)(κ^2-*S,N*-C_6H_4CS=N-(2-ClPh)(PPh_3)] (2a)	$C_{30}H_{23}Cl_2N_2PPdS$	55.27(55.09)	3.56(3.54)	4.30(4.28)	4.92(4.90)
[Pd(Cl)(κ^2-*S,N*-C_6H_4CS=N-(2-MePh)(PPh_3)] (2b)	$C_{31}H_{26}ClN_2PPdS$	58.96(58.81)	4.15(4.17)	4.44(4.46)	5.08(5.05)
[Pd(Cl)(κ^2-*S,N*-C_6H_4CS=N-(4-MePh)(PPh_3)] (2c)	$C_{31}H_{26}ClN_2PPdS$	58.96(59.10)	4.15(4.18)	4.44(4.42)	5.08(5.09)
[Pd(Cl)(κ^2-*S,N*-C_6H_4CS=N-(4-Py)(PPh_3)] (2d)	$C_{29}H_{23}ClN_3PPdS$	56.32(56.17)	3.75(3.72)	6.79(6.76)	5.18(5.18)

Table S2: Selected IR spectral data of Pd(II) thiocarboxamide complexes

Complexes	$\nu_{(C-S)}$ (cm^{-1})	$\nu_{(C=N)}$ (cm^{-1})
2a	1281	1562
2b	1275	1545
2c	1267	1549
2d	1277	1553

Table S3: ^{1}H & ^{31}P NMR spectral data of Pd(II) thiocarboxamide complexes

Complexes	^{1}H NMR data (ppm)			^{31}P NMR data (ppm)
	Ar–H (t)(1-H)	Ar–H, PPh_3 (m)	CH_3 (s)	PPh_3 (s)
2a	9.58(d)	7.65-7.25	-	30.76
2b	9.58	7.93-6.86	2.10	31.03
2c	9.79	7.89-6.99	2.25	30.92
2d	9.59	8.34-6.85	-	30.59

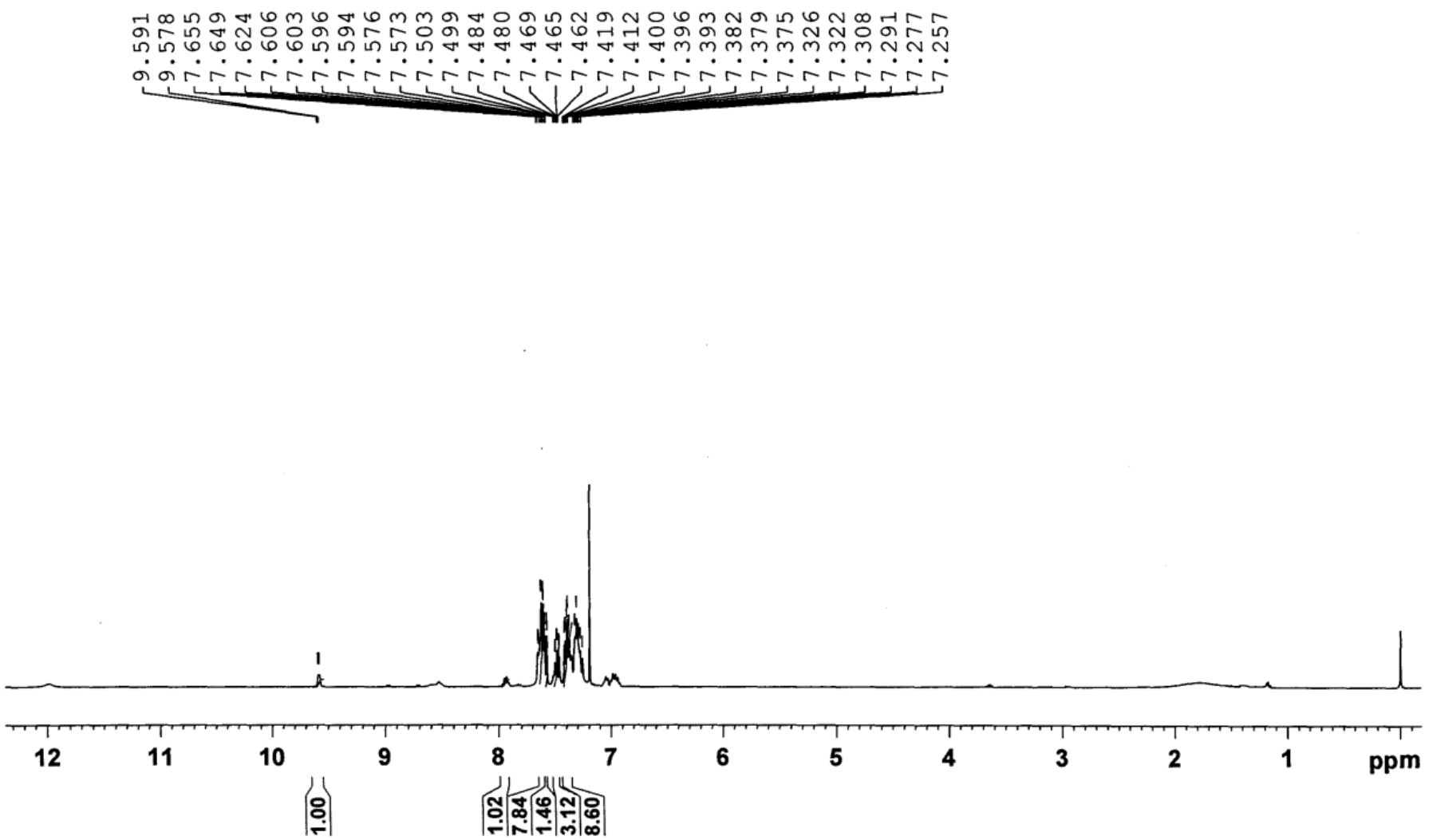

Figure S1: ^{1}H NMR for Pd(II) thiocarboxamide Complex **2a**

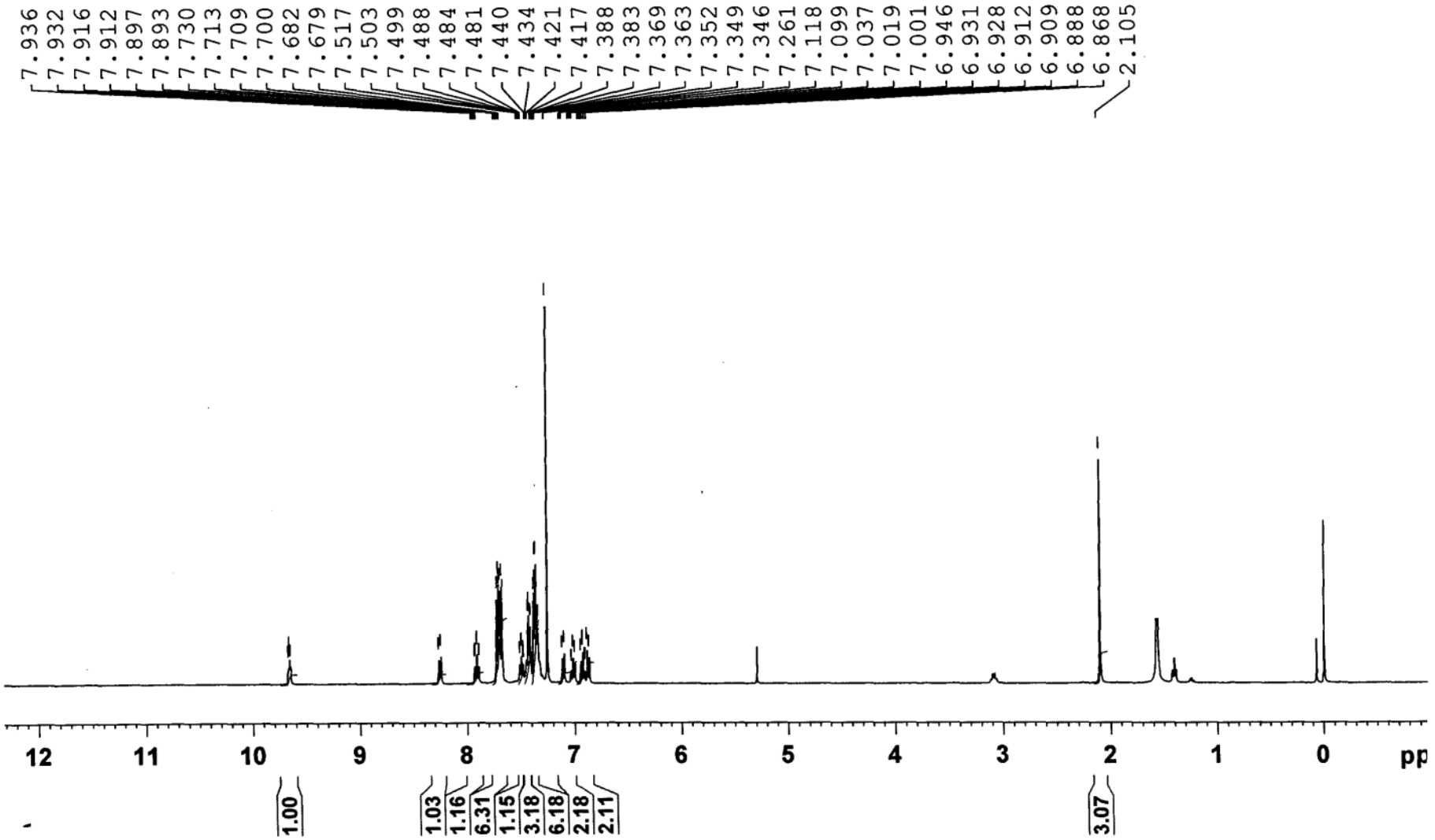

Figure S2: ^{1}H NMR for Pd(II) thiocarboxamide Complex **2b**

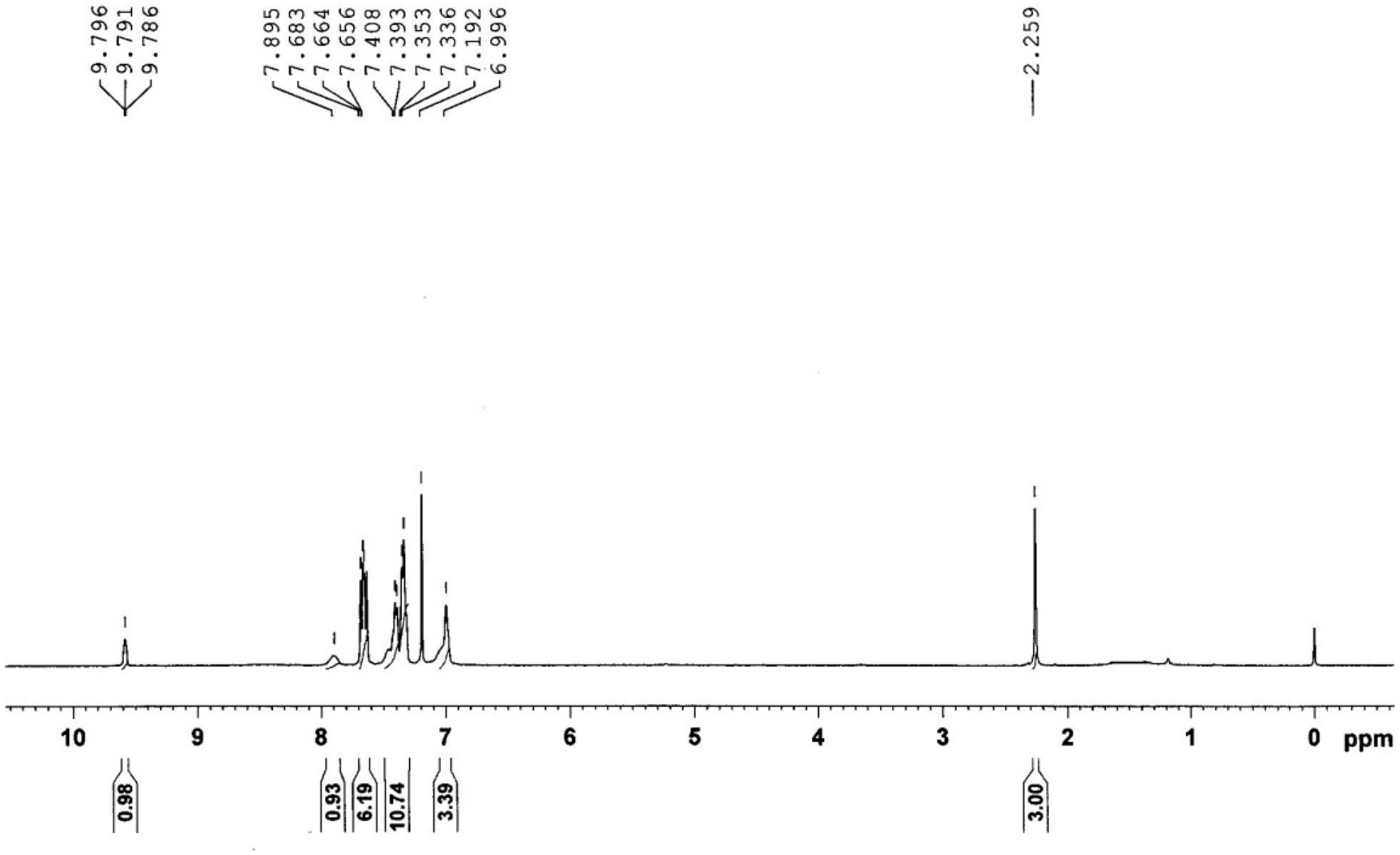

Figure S3: ^{1}H NMR for Pd(II) thiocarboxamide Complex **2c**

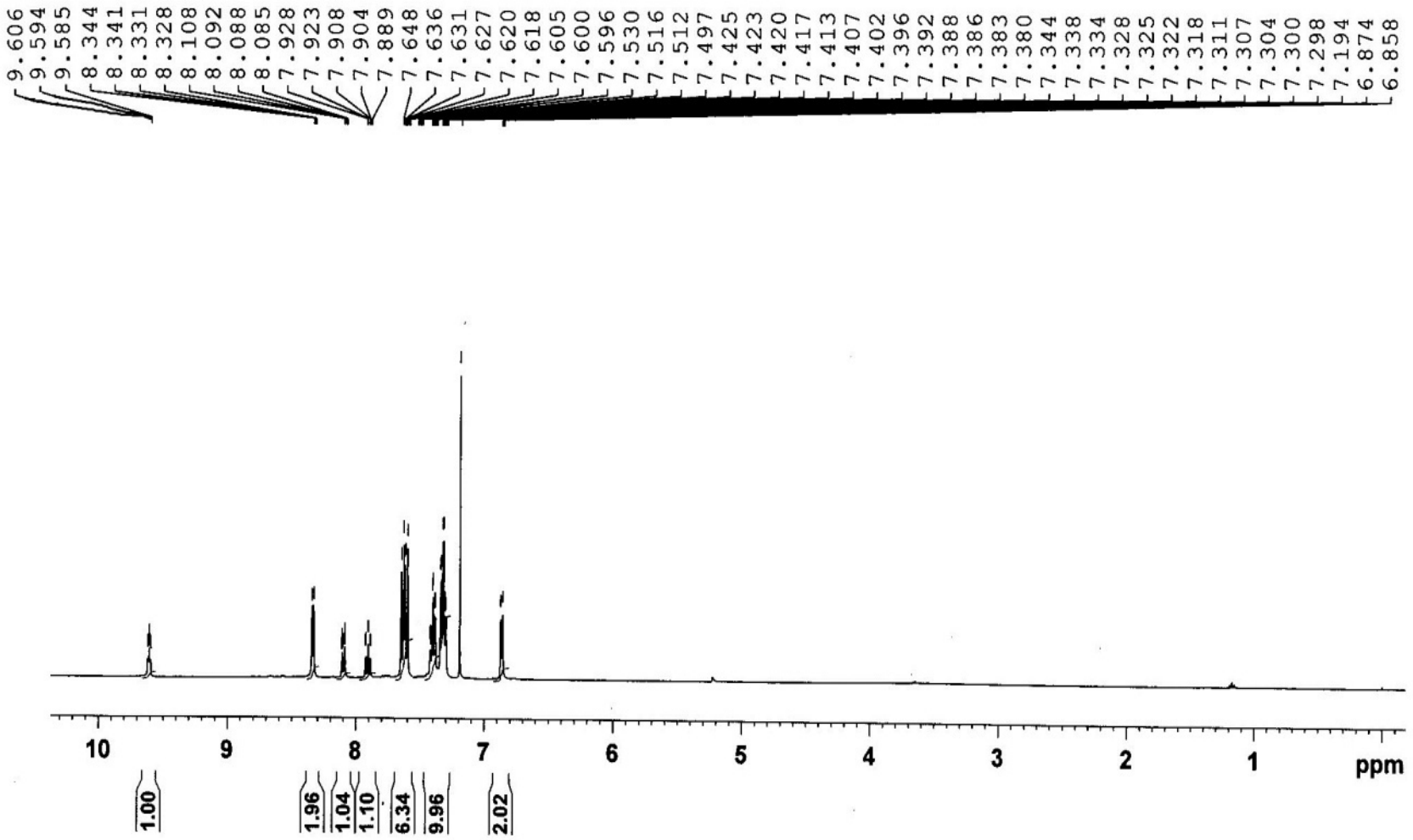

Figure S4: ^{1}H NMR for Pd(II) thiocarboxamide Complex **2d**

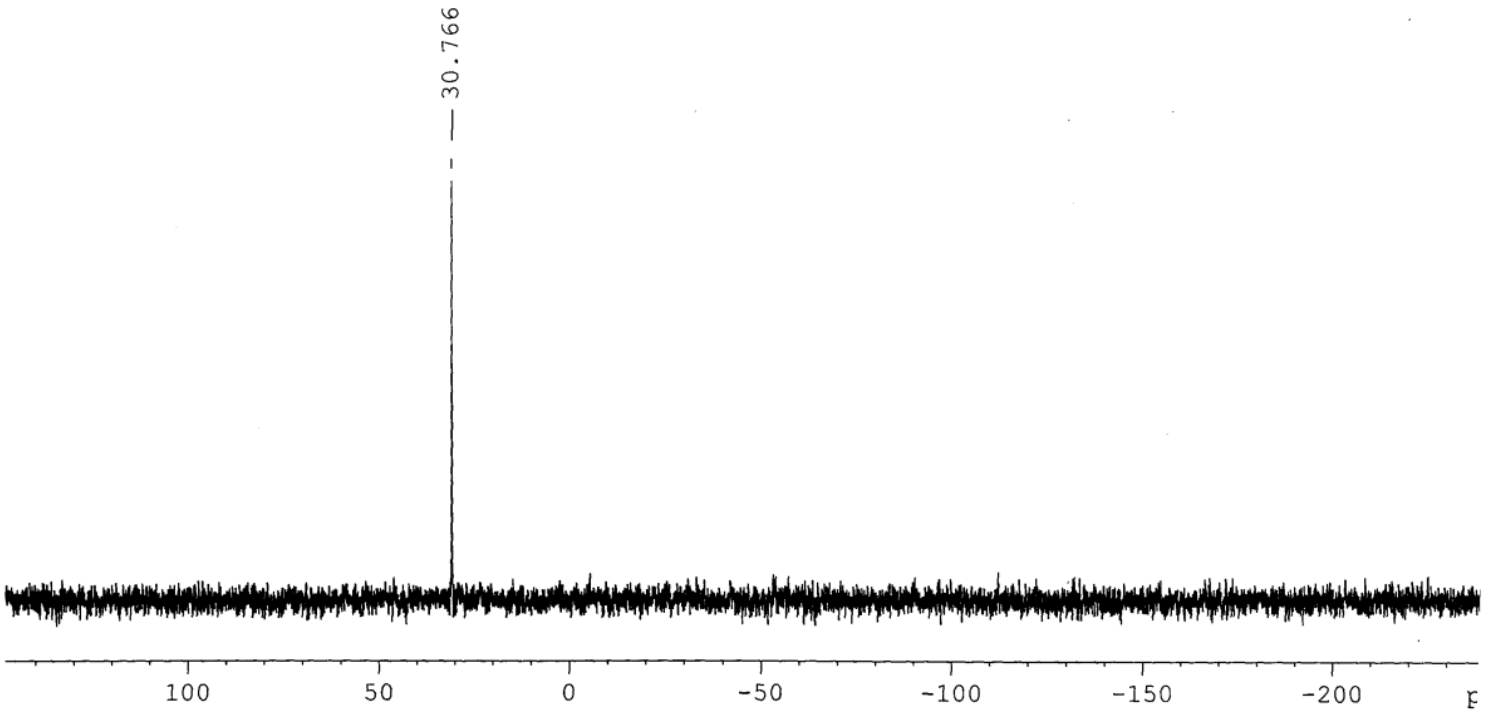

Figure S5: ^{31}P NMR for Pd(II) thiocarboxamide Complex **2a**

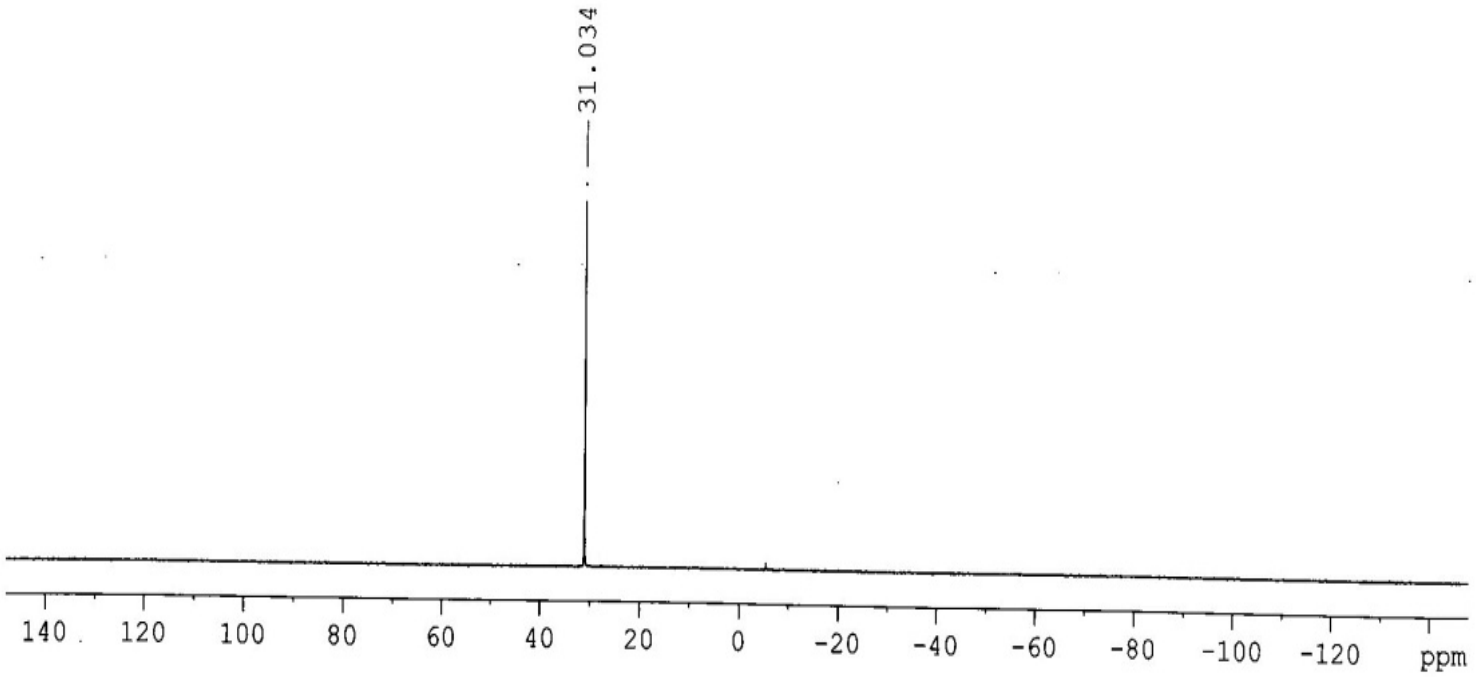

Figure S6: ^{31}P NMR for Pd(II) thiocarboxamide Complex **2b**

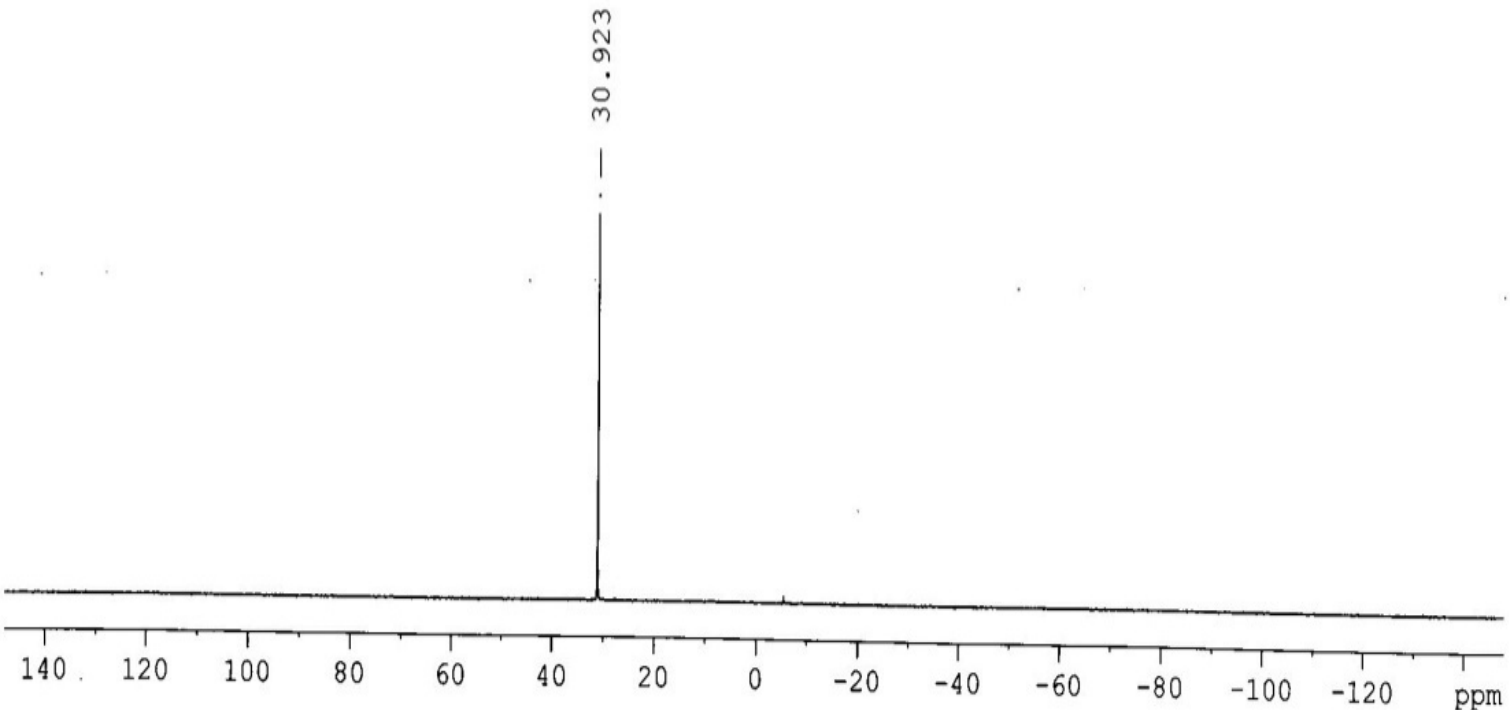

Figure S7: ^{31}P NMR for Pd(II) thiocarboxamide Complex **2c**

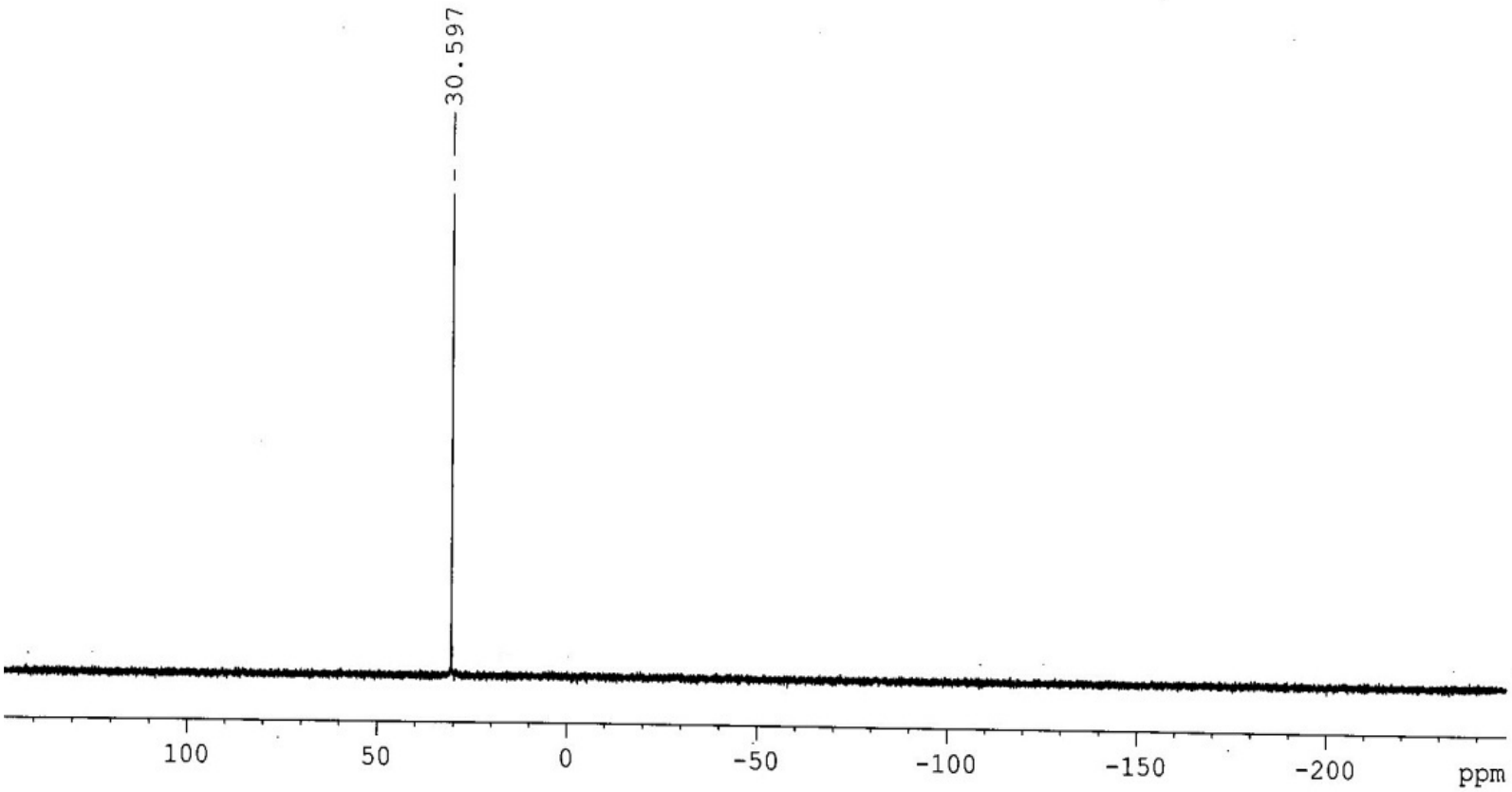

Figure S8: ^{31}P NMR for Pd(II) thiocarboxamide Complex **2d**

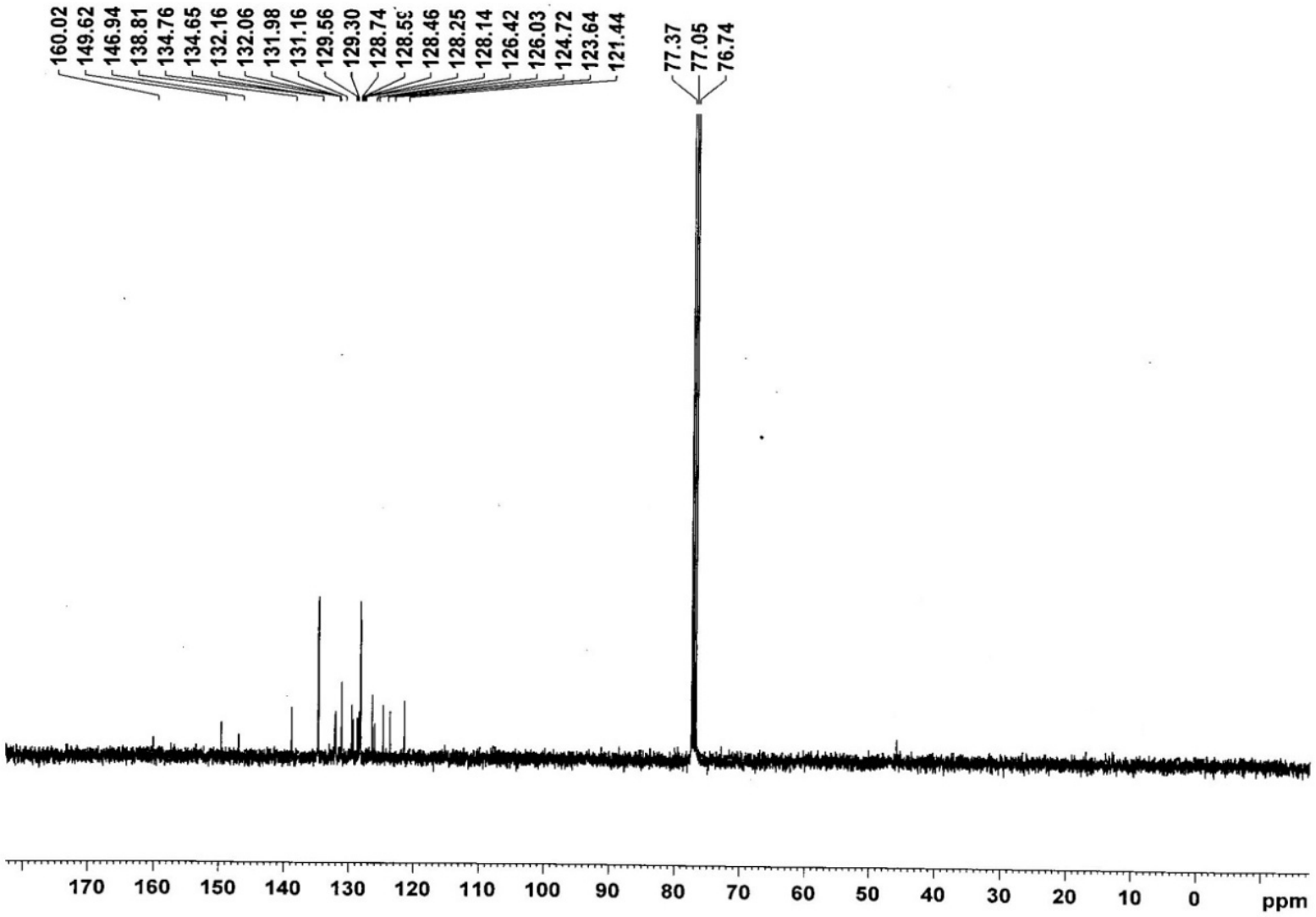

Figure S9: ^{13}C NMR for Pd(II) thiocarboxamide Complex **2a**

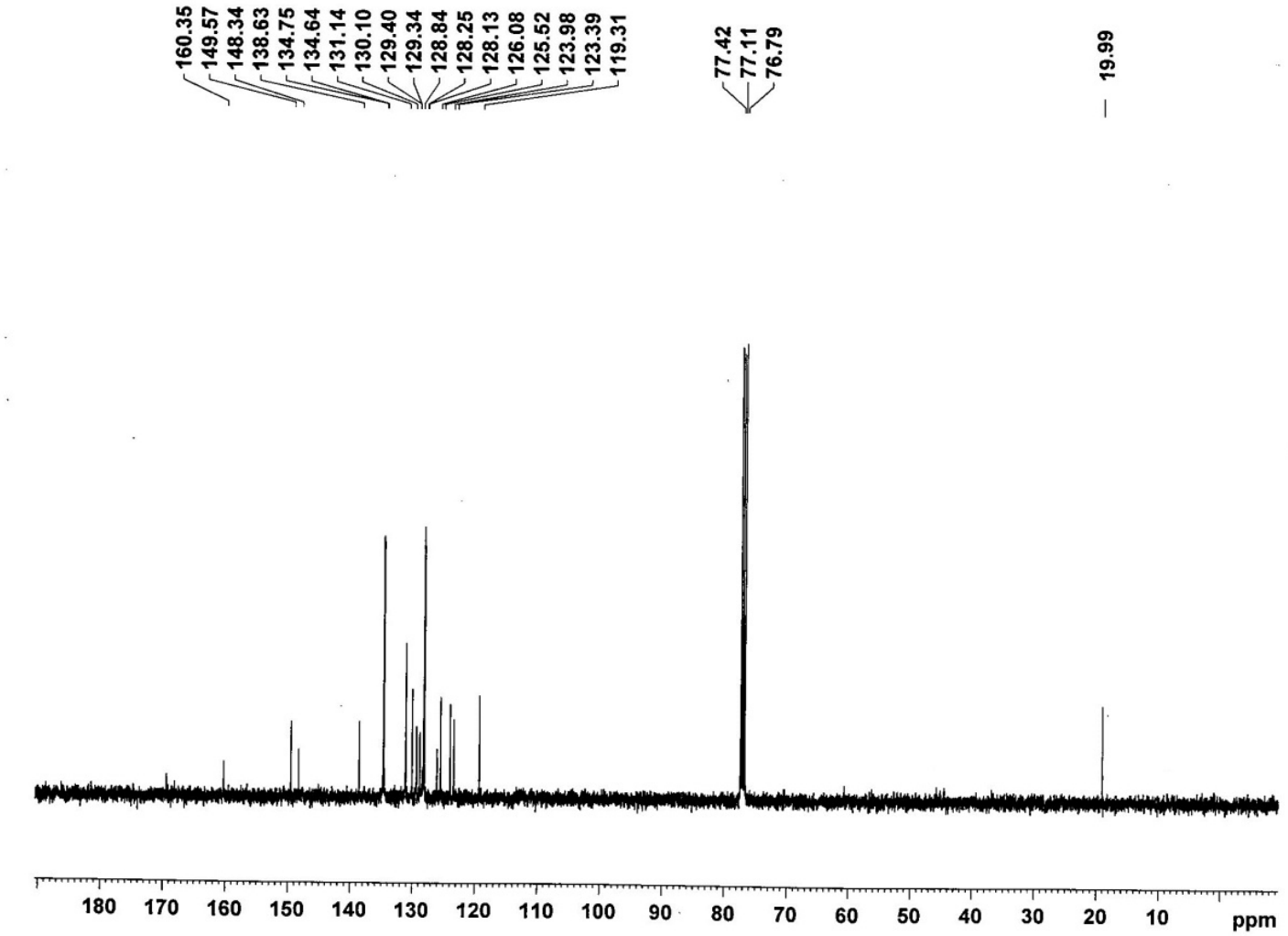

Figure S10: ^{13}C NMR for Pd(II) thiocarboxamide Complex **2b**

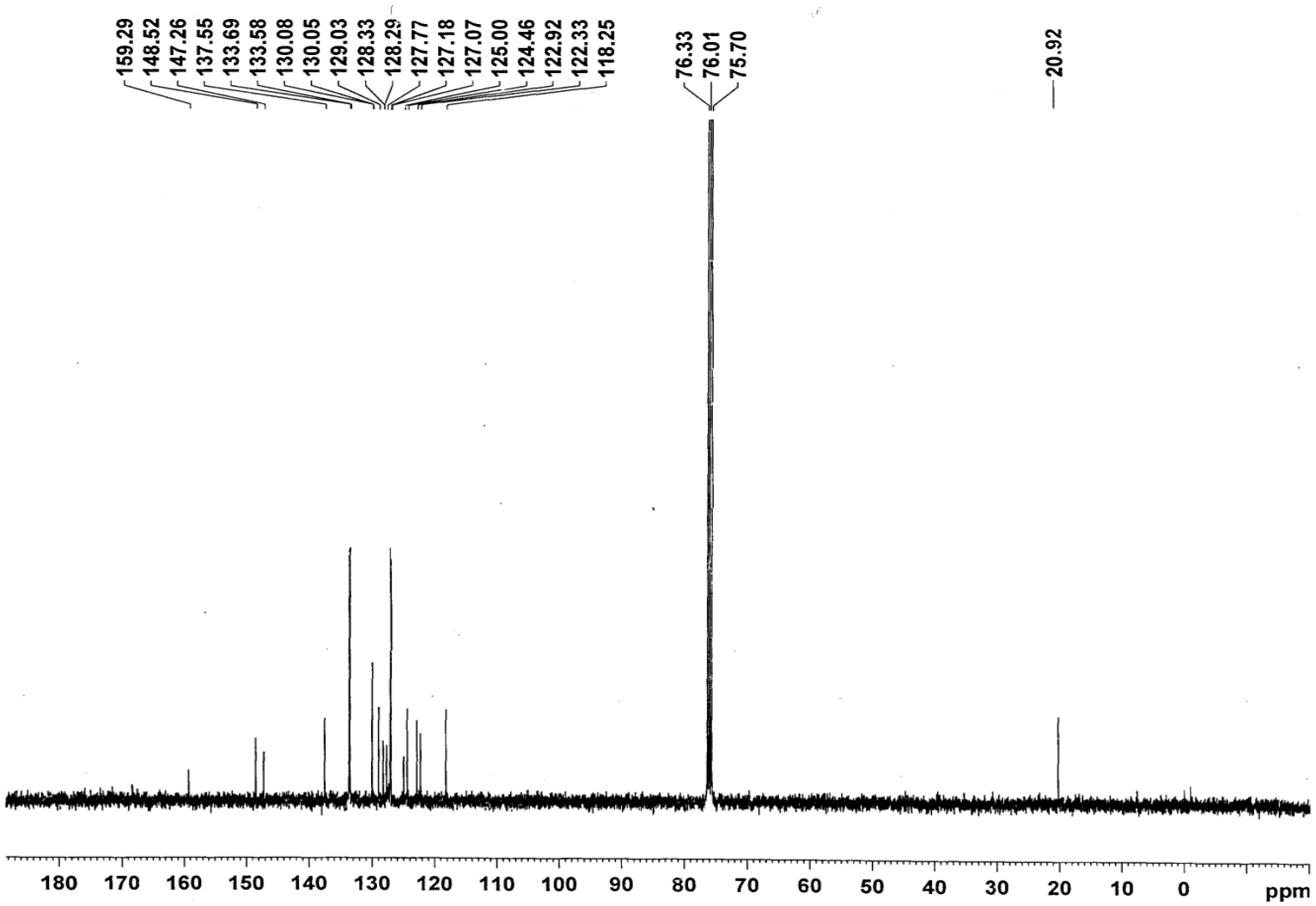

Figure S11: ^{13}C NMR for Pd(II) thiocarboxamide Complex **2c**

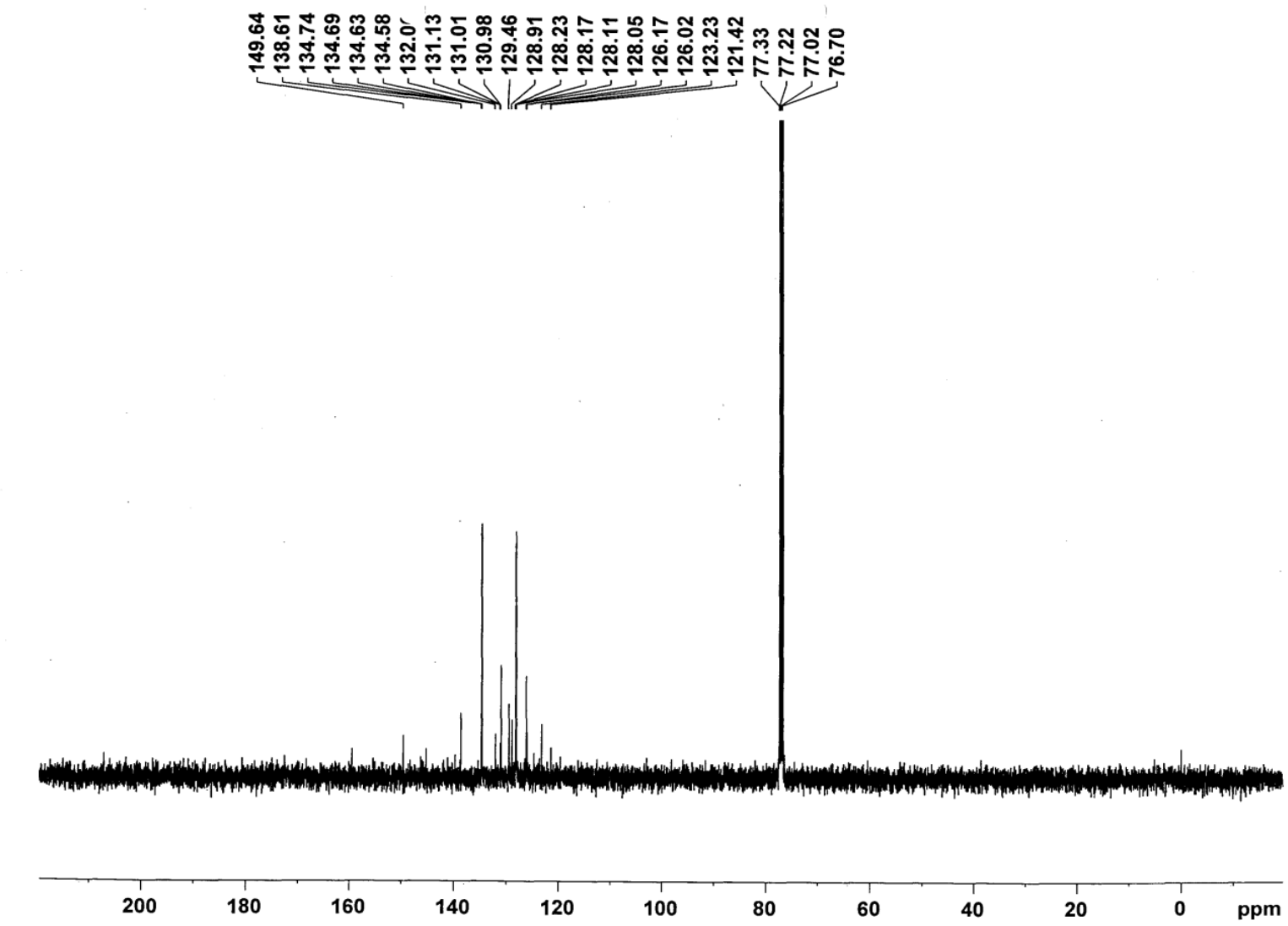

Figure S12: ^{13}C NMR for Pd(II) thiocarboxamide Complex **2d**